Structural Causal Models and Abstraction for Modeling Battery Manufacturing

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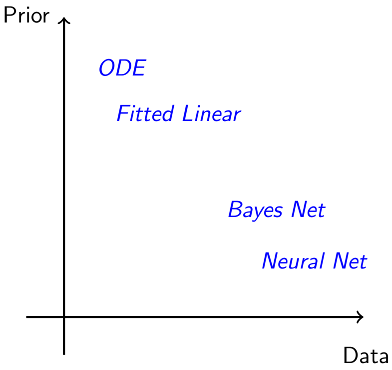
Outline

2. Structural Causal Modelling

Modelling

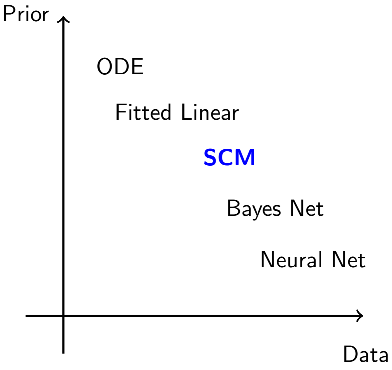
Assume we want to model a *system*.

Different types of model will negotiate a trade-off between priors and data:



Structural Causal Models

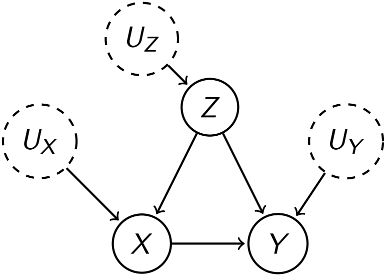
Structural causal models rely on a strong prior given by *causality* [5].



- It discriminates *correlations* and *causes*.
- It allows for reasoning about *interventions*.
- It allows for reasoning about *counterfactuals*.
- It implies a *causality ladder* of reasoning.
- It requires more than data.

Structural causal model

A **SCM** [4, 5] is a mathematical object $\mathcal{M} = \langle \mathcal{X}, \mathcal{U}, \mathcal{F}, \mathcal{P} \rangle$ with an associated DAG:

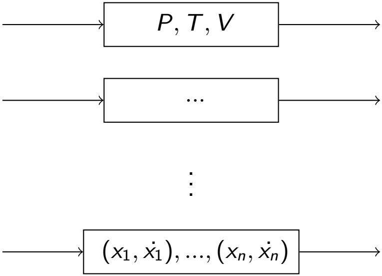


- It adds *structure* to a purely statistical model.
- It does not require to be *fully defined*.
- It allows for *causal inference* [4, 8] and *causal discovery* [3] relying on data.

3. Abstraction

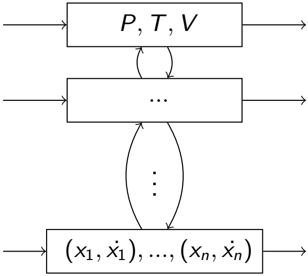
Modelling

A system can be modelled on multiple *levels of abstraction*.



Abstraction

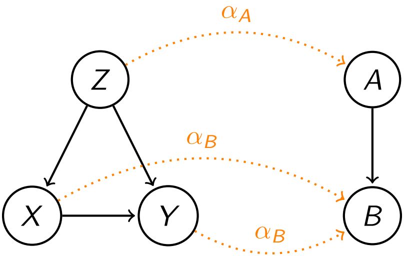
Abstraction (aka, *multi-level modelling* or *multi-resolution modelling*) aims at relating these levels.



- It combines models from *different sources*.
- It aggregates information from *different resolutions*.
- It allows for *computation with minimal effort*.

Causal Abstraction

Causal abstraction is a collection of maps α between two SCMs $\mathcal{M}$ and $\mathcal{M}'$ that relates variables [7, 1, 6].



- It captures *coarsening/change of resolution/simplification of structure*.

Causal Consistency

We impose on the *causal abstraction* a requirement of *interventional consistency* (or *approximate interventional consistency*) [7, 1, 6].

$$\begin{tikzcd} \mathcal{M} \arrow[r, "\alpha"] \arrow[d, "\iota"'] & \mathcal{M}' \arrow[d, "\iota'"] \\ \mathcal{M}_\iota \arrow[r, "\alpha"] & \mathcal{M}'_{\iota'} \end{tikzcd}$$

- Consistency would allow to *switch*/*intergrate* models.
- We have a *formal definition*, limited methodology.

Recap

With **causality** we can:

- Exploit (partial) prior causal knowledge to define causal DAG
- Exploit (partially defined) DAGs to perform causal inference

With **causal abstraction** we can:

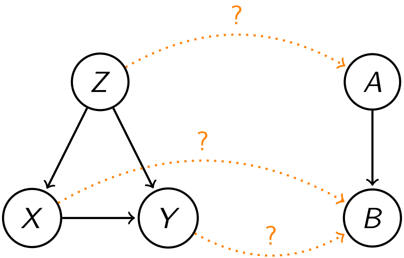
- Exploit causal models at multiple levels to leverage heterogeneous data

- *How do we learn an abstraction if we are not given one?*
- *How do we apply it to the relevant problem of battery manufacturing?*

4. Learning Causal Abstractions

Learning Causal Abstraction

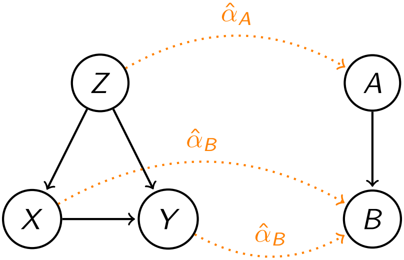
How do we learn the abstraction maps?



- Not trivial: we have to deal with a *combinatorial optimization* problem for each map α_i.
- Optimization of the maps with respect to global consistency introduces *dependencies*.

Jointly Learning Causal Abstraction

We have proposed a first methodology to learn an abstraction.



- It relies on *relaxing* the problem and using *differentiable programming* to learn all maps at once.
- *Heuristic* - highly efficient at the cost of sub-optimality.
- It requires substantial *prior* knowledge (SCM).

5. Modelling Battery Manufacturing

Problem Definition

We want to model the stage of **coating** in lithium-ion battery manufacturing:

$$\text{Mass Loading} = \text{f(input)}$$

Experiments are costly, so we want to integrate data[1] collected by two groups running similar (but not identical) experiments:

LRCS (France)	**WMG** (UK)
Collection of few statistics in each a few stages of battery manufacturing [2].	Collection of detailed space- and time-dependent measurements during coating.

[1] `https://chemistry-europe.onlinelibrary.wiley.com/doi/full/10.1002/batt.201900135`
`https://github.com/mattdravucz/jointly-learning-causal-abstraction/`

Datasets

LRCS

- *Input params:* AM composition, S-to-L ratio, comma gap, viscosity.
- *Output params:* mass loading, porosity
- 656 datapoints in 82 configurations.

high-level, wide

WMG

- *Experimental params:* AM composition, ...
- *Machine params:* Comma bar operator position actual, Coating roll gear ratio setpoint, ... measured every 1s
- *Output params:* Mass loading ... measured every 8s at 800 spatial locations
- 1 experiment lasting 3h with varying configurations

low-level, narrow

Preprocessing and alignment

LRCS

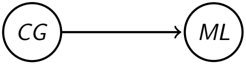
- Unit conversion
  Aligning unit of measure
- Params subselection
  Dropping slurry params
- Discretization
  Binning ML into n_{bins}

WMG

- Params combination
  Reconstructing actual comma gap
- Time subselection
  Filtering transitions and downtimes
- Space averaging
  From 800 locations to n_{loc}
- Discretization
  Binning ML into n_{bins}
- Data Extraploation
  Additional CG values via GPs

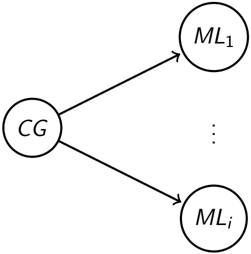
SCM definition

LRCS



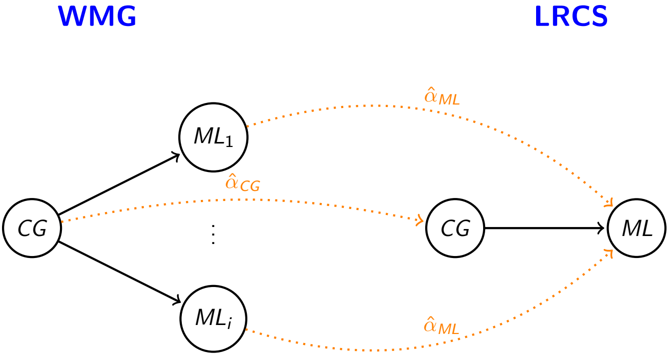
$$\mathcal{M}^{LRCS}[CG] = \{75, 100, 200\}$$
$$\mathcal{M}^{LRCS}[ML] = \{0, 1, ..., n_{bins}\}$$

WMG



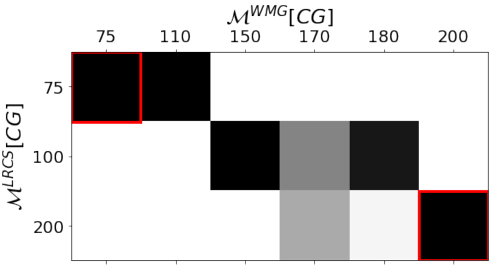
$$\mathcal{M}^{WMG}[CG] = \{75, 110, 150, 170, 180, 200\}$$
$$\mathcal{M}^{WMG}[ML_i] = \{0, 1, ..., n_{bins}\}$$

Learning abstraction



- *Jointly learning causal abstraction*
- Explored a small number of hyperparameters (T, η, λ) across 50 instances.

Results: Insight



- Learning achieves meaningful results *based only on probabilistic and interventional behaviour* (with no reference to semantics).
- Variability remains a challenge

Results: Downstream task

How does aggregation of data really perform on actual problems?

Out-of-sample prediction: LRCS use a LASSO model to predict ML as a function of $CG = k$, when $CG = k$ is far from the training set.

	Training set	**Test Set**	**MSE**
(a)	LRCS[$CG \neq k$]	LRCS[$CG = k$]	1.86 ± 1.75
(b)	LRCS[$CG \neq k$] + WMG	LRCS[$CG = k$]	0.22 ± 0.26
(c)	LRCS[$CG \neq k$] + WMG[$CG \neq k$]	LRCS[$CG = k$] + WMG[$CG = k$]	1.22 ± 0.95

- Transferring data can increase statistical power

Conclusion

- *Causality* and *abstraction* may both play important role in modelling.
- This is first proposal for *learning abstraction*.
- Preliminary results show promise for *combining* diverse data and take advantage of it.

Thanks!

Thank you for listening!

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[1] Sander Beckers and Joseph Y Halpern. Abstracting causal models. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 33, pages 2678–2685, 2019.

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